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EDITOR'S NOTE

With the exception of certain trigonometric and hyperbolic functions, Soviet mathematical symbols are the same as those encountered in the American literature. For the reader's convenience a list of such exceptions and their American equivalents is given below.

Soviet Usage	American equivalent
Arch	$\cosh^{-1}$
Arcth	$\coth^{-1}$ (ctnh^{-1})
Arsh	$\sinh^{-1}$
Arth	$\tanh^{-1}$
arccos	$\cos^{-1}$ (arc cos)
arcctg	$\cot^{-1}$ (arc cot)
arcsin	$\sin^{-1}$ (arc sin)
arctg	$\tan^{-1}$ (arc tan)
ch	cosh
cosec	csc
ctg	cot (ctn)
cth	coth (ctnh)
rot	curl
sch	sech
sh	sinh
tg	tan
th	tanh

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Several difference schemes [1-4] for numerical solution of three-dimensional supersonic gas-dynamic problems have been developed in recent years and used in various applications. These are based on the use of the characteristic compatibility relations. Among these schemes, an especially simple one is the numerical scheme of the semi-characteristic type [1], in which one independent variable associated with the transverse flow is excluded by means of appropriate approximations and the problem is in fact reduced to integration of a two-dimensional hyperbolic system of equations. In the article [1], such a semi-characteristic scheme was developed for calculation of three-dimensional supersonic equilibrium gas flow about a body located at the angle of attack. The application of this scheme both to blunted bodies [5] and to bodies incorporating a channel [6] of sufficiently smooth form has pointed to its efficiency. This semi-characteristic scheme was generalized [7] (see also [8]) to the case of three-dimensional gas flows accompanied by nonequilibrium physical and chemical processes. In the present article the computational algorithms of that scheme are given in detail for such case, in particular, to its application for numerical solution of supersonic flow of nonequilibrium dissociating oxygen in a nonaxisymmetric nozzle. /1049*

1. The system of equations for nonequilibrium gas flows

We take the general equations of gasdynamics (the equation of continuity, the equation of conservation of momentum, and the equation of conservation of energy) for steady-state three-dimensional flow of a nonviscous, thermally nonconducting gas

$$\nabla \rho \mathbf{V} = 0, \quad \rho (\mathbf{V}\nabla)\mathbf{V} + \nabla p = 0, \quad \rho \mathbf{V}\nabla h - \mathbf{V}\nabla p = 0, \tag{1.1}$$

where V is the velocity vector, p is the pressure, ρ is the density, and h is the specific enthalpy.

As is known [9, 10], the course of nonequilibrium physicochemical processes in a gas can be described by the variation of certain parameters c_i (for i = 1, 2, ..., m), which can be, for example, the energies of the internal degrees of freedom, the mass concentrations, etc. Other governing physical parameters are the pressure p and the temperature T of the translational degrees of freedom of one of the components. Then, the equation of state and the expression for the enthalpy can be analyzed as the relationships /1050

*Numbers in the margin indicate pagination in the foreign text.

$$\rho = \rho(p, T, c_1, c_2, \ldots, c_m), \qquad h = h(p, T, c_1, c_2, \ldots, c_m), \tag{1.2}$$

The starting system of equations is completed by the equations for the parameters c_i, which are the total derivatives with respect to time

$$\frac{dc_i}{dt} = F_i(p, T, c_1, c_2, \ldots, c_m) \qquad (i = 1, 2, \ldots, m). \tag{1.3}$$

The right-hand members of these equations have the following structure:

$$F_i = \varphi_i(p, T, c_1, c_2, \ldots, c_m) f_i(p, T, c_1, c_2, \ldots, c_m), \tag{1.4}$$

or, in the more general case, they consist of several terms of this form. Here, the function φ_i is proportional to the rate of the physicochemical process. For a flow with "frozen in" reactions, $\varphi_i = 0$. For a flow with equilibrium reactions, /1050 $\varphi_i \to \infty$ and, in this case, $f_i = 0$. The specific form of (1.3) and that of (1.2) is determined by the physical and the chemical kinetics.

We shall use dimensionless variables, taking as the characteristic quantities some linear dimension, the velocity V_∞ and density ρ_∞ of the unperturbed flow, and the gas constant. The characteristic quantities for the parameters c are chosen in accordance with their physical meaning.

In solving the problems of the flow of a gas, we shall confine ourselves (for simplicity) to non-axisymmetric bodies, the cross-sections of which do not differ greatly from ellipses, and which possess one plane of symmetry parallel to the unperturbed flow. In this case, it is convenient to use the coordinates x, ξ, η, with the x-axis passing through the body in the longitudinal direction (for a body of rotation, it coincides with the axis of rotation), the surface ξ = constant are elliptic, and the surfaces η = const are hyperbolic. In the problem of a flow around a body at the angle of attack, we may assume that the value $\eta = 0$ corresponds to the windward side and $\eta = \pi$ to the leeward.

On this system of equations we impose definite boundary conditions. Suppose that the region of flow has boundary surfaces $\xi = \xi_B(x, \eta)$ and $\xi = \xi_T(x, \eta)$. In the case of external flow around the body, the first surface is the shock wave and the second is the surface of the body. On the other hand, in the case of internal flow in the nozzle, these surfaces will be, respectively, the wall of the nozzle and its axis, or the surface of the internal profiled body (for an annular nozzle).

If the boundary is an impenetrable wall $\xi = \xi_T(x, \eta)$, then the normal velocity on it vanishes, which yields the condition

$$\xi_{Tx}' u + v + \xi_{T\eta}' w = 0, \tag{1.5}$$

where u, v, and w denote the components of the velocity along the x-, ξ-, and η-axes respectively.

On the other hand, if the boundary is a shock wave, the gasdynamic conditions existing on a sharp discontinuity must be satisfied on it. A shock wave is an infinitely thin surface; therefore, the parameters c_i describing the physicochemical processes stay constant upon traversal of that front. Consequently, the values of the gasdynamic functions immediately behind the shock wave will, in nonequilibrium flow, be found in the same way as in the case of flow with "frozen in" reactions. In the case of uniform supersonic (Mach M_∞) flow around a body, where the angle of incidence α to the x-axis is the angle of attack, these values are expressed by the formulas

$$p = p_\infty + \Delta p, \qquad \Delta p = \left(1 - \frac{1}{\rho}\right) V_{n\infty}^2,$$

$$h = h_\infty + \frac{\Delta p}{2}\left(1 + \frac{1}{\rho}\right), \qquad u = \cos\alpha - \frac{\Delta p H \xi_{Bx}'}{\delta}, \tag{1.6}$$

$$v = -\sin\alpha \frac{\operatorname{ch}\xi\cos\eta}{H} + \frac{\Delta p}{\delta}, \qquad w = \sin\alpha \frac{\operatorname{sh}\xi\sin\eta}{H} - \frac{\Delta p}{\delta}\xi_{B\eta}',$$

where the Lamé parameter (half the focal distance is taken as the characteristic linear dimension) is equal to $H = (\operatorname{sh}^2\xi + \sin^2\eta)^{1/2}$ and the component of velocity of unperturbed flow normal to the shock wave is

$$V_{n\infty} = \delta(1 + H^2\xi_{Bx}'^2 + \xi_{B\eta}'^2)^{-1/2},$$

where

$$\delta = H\xi_{Bx}'\cos\alpha + \frac{\operatorname{ch}\xi\cos\eta}{H}\sin\alpha + \frac{\operatorname{sh}\xi\sin\eta}{H}\xi_{B\eta}'\sin\alpha.$$

In the non-equilibrium case, it is necessary to take into account (1.2) which, generally speaking, are complex even for constant parameters c_i on the shock wave. Therefore, determination of the functions from (1.6) for given values of the derivatives ξ_{Bx}' and $\xi_{B\eta}'$ necessitates the use of iteration. For example, we may use Newton's method and carry out the iterations with respect to the quantity ρ, solving the first three equations in (1.6), as well as (1.2), and finding as a result the values of p, h, T, and ρ.

In the calculation of the supersonic flow, the initial values of the basic unknown functions on some space-type surface must also be given.

In the investigation of gas nonequilibrium flows let us consider the "frozen in" sound velocity

$$a = \left[\rho_p' + \frac{\rho_T'}{h_T'}\left(\frac{1}{\rho} - h_p'\right)\right]^{-1/2}, \tag{1.7}$$

where the prime denotes the partial derivative with respect to the variable indicated by the subscript. At supersonic velocity, the system of equations (1.1)-(1.3) will be hyperbolic. Then, at every point of the three-dimensional flow region there will exist a one-parameter family of characteristic surfaces, the envelope of which is the characteristic conoid. The characteristic surfaces are determined by those terms in (1.1) that contain partial derivatives. Therefore, their equations will be identical in the equilibrium and nonequilibrium cases. /1052

Of course, there will be certain differences in the characteristic compatibility relations. Let us consider, at a given point, the characteristic plane with a unit external normal n tangent to the conoid. By using the work of [11], we can obtain, in the case of steady-state nonequilibrium flow, the characteristic compatibility relation in the form

$$\rho a A_2 d_{s_1} V - B_2 d_{s_1} p = \rho a A_1 d_{s_2} V - B_1 d_{s_2} p + \Omega n (s_1 \times s_2).$$

Here,

$$A_j = V \times s_j, \quad B_j = nA_j, \quad \Omega = a^2 \sum_{i=1}^{m} \left(\rho_{c_i}' - \rho_{T'} \frac{h_{ci}'}{h_{T'}} \right) F_i,$$

and s_1 and s_2 are two independent vectors lying in the characteristic plane under consideration.

The streamline is an (m + 3) triple characteristic. Along it, there hold m equations (1.3) describing the physicochemical transformations. Furthermore, the Bernoulli equation $V^2/2 + h = \text{const}$ and the equation of energy in (1.1) are satisfied on a streamline that equation of energy can, by virtue of (1.2), be transformed to

$$dT + g dp + q dt = 0, \tag{1.8}$$

where

$$g = \frac{1}{h_{T'}} \left(h_{p'} - \frac{1}{\rho} \right), \qquad q = \frac{1}{h_{T'}} \sum_{i=1}^{m} h_{ci}' F_i.$$

These characteristic relations enable us to construct various numerical schemes of the three-dimensional method of characteristics for calculating three-dimensional supersonic nonequilibrium flows and, in particular, to generalize schemes [2-4] to this case. However, as already noted, we shall construct here a numerical scheme by use of two-dimensional characteristic relationships. We shall begin by reducing the initial system of equations to a system with two independent variables.

2. The approximating system of equations

From the system of equations (1.1)-(1.3), which have three variables, we derive the approximating two-dimensional system. First of all, we transform the equation of continuity in (1.1) with the aid of the other equations of the system as follows:

$$\rho a^2 \nabla \mathbf{V} + \mathbf{V} \nabla p + \Omega = 0. \tag{2.1}$$

Then, (2.1), the equation of momentum in (1.1), the equation of energy (1.8), and the kinetic equations (1.3) become the initial three-dimensional equations for the functions V, p, T, and c_i.

To rectify the region of flow bounded by surfaces $\xi = \xi_T(x, \eta)$ and $\xi = \xi_B(x, \eta)$, we introduce the normalized variable $\vartheta = (\xi - \xi_T)\varepsilon^{-1}$, in place of ε; here $= \xi_B - \xi_T$. Let us write the equations enumerated above in terms of the variables x, ϑ, η. /1053

We now eliminate from these equations the variable η, by using in the region $0 \leqslant \eta \leqslant \pi$ the trigonometric interpolational polynomials in which the interpolational nodes are the surfaces $\eta = \eta_k = k\pi / l$ (for k = 0, 1, ..., l). For an odd function w and even functions $\mathcal{F}$, we take respectively the approximations

$$w = \sum_{k=1}^{l-1} \sum_{j=1}^{l-1} c_{kj} w_j \sin k\eta, \quad \mathcal{F} = \sum_{k=0}^{l} \sum_{j=0}^{l} d_{kj} \mathcal{F}_j \cos k\eta. \tag{2.2}$$

From these we determine the derivatives

$$\left(\frac{\partial w}{\partial \eta}\right)_k = \sum_{j=1}^{l-1} e_{kj} w_j, \quad \left(\frac{\partial \mathcal{F}}{\partial \eta}\right)_k = \sum_{j=0}^{l} f_{kj} \mathcal{F}_j. \tag{2.3}$$

Here, the subscripts in the expressions for the functions and the derivatives indicate values relating to the corresponding surface η = const. The numerical coefficients c_{kj} and d_{kj} are found from the formulas

$$c_{kj} = 2l^{-1} \sin k\eta_j, \quad d_{kj} = 2l^{-1} \cos k\eta_j,$$

When k = 0 and when k = 1, we need to replace factor 2 in the formula for d_{kj} by factor 1 at $0 < j < l$, and by factor 1/2 at j = 0 and j = l. One can also easily calculate the numerical coefficients e_{kj} and f_{kj} for l = 2, 3, 4. All these coefficients are given in [1].

Thus, with the aid of the representations (2.2), we obtain a two-dimensional approximating system whose form $\eta = \eta_k$ on each surface of interpolation (henceforth we shall, for simplicity, drop the subscript k) is

$$\frac{\partial u}{\partial x}+\frac{1}{\varepsilon}\left(\lambda\frac{\partial u}{\partial\vartheta}+\frac{\partial v}{H\partial\vartheta}+\frac{\mu}{H}\frac{\partial w}{\partial\vartheta}\right)+\frac{1}{\rho a^2}\left(u\frac{\partial p}{\partial x}+v\frac{\partial p}{\partial\vartheta}\right)+\Phi_1=0,$$

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial\vartheta}+\frac{1}{\rho}\left(\frac{\partial p}{\partial x}+\frac{\lambda}{\varepsilon}\frac{\partial p}{\partial\vartheta}\right)+\Phi_2=0,$$

$$u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial\vartheta}+\frac{1}{\rho He}\frac{\partial p}{\partial\vartheta}+\Phi_3=0,\qquad u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial\vartheta}+\frac{\mu}{\rho He}\frac{\partial p}{\partial\vartheta}+\Phi_4=0,$$

$$\frac{1}{h_T'}\left(h_p'-\frac{1}{\rho}\right)\left(u\frac{\partial p}{\partial x}+v\frac{\partial p}{\partial\vartheta}\right)+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial\vartheta}+\Phi_5=0,$$

$$u\frac{\partial c_i}{\partial x}+v\frac{\partial c_i}{\partial\vartheta}+\Phi_{5+i}=0\qquad(i=1,2,\ldots,m),$$

where

$$\lambda=\vartheta(\xi'_{\tau x}-\xi'_{nx})-\xi'_{\tau x},\quad \mu=\vartheta(\xi'_{\tau\eta}-\xi'_{n\eta})-\xi'_{\tau\eta},$$

$$v=\frac{1}{\varepsilon}\left(\lambda u+\frac{v}{H}+\frac{\mu w}{H}\right),\quad \sigma=\frac{\operatorname{sh}\xi\operatorname{ch}\xi}{H^3},\quad \tau=-\frac{\sin\eta\cos\eta}{H^3}$$

$$\Phi_1=\sigma v+\tau w+\frac{1}{H}\left(\frac{\partial w}{\partial\eta}+\frac{w}{\rho a^2}\frac{\partial p}{\partial\eta}\right)+\frac{\Omega}{\rho a^2},\quad \Phi_2=\frac{w}{H}\frac{\partial u}{\partial\eta},$$

$$\Phi_3=w(\tau v-\sigma w)+\frac{w}{H}\frac{\partial v}{\partial\eta},\quad \Phi_4=-v(\tau v-\sigma w)+\frac{w}{H}\frac{\partial w}{\partial\eta}+\frac{1}{H\rho}\frac{\partial p}{\partial\eta},$$

$$\Phi_5=\frac{w}{H}\left(g\frac{\partial p}{\partial\eta}+\frac{\partial T}{\partial\eta}\right)+q,\quad \Phi_{5+i}=W_i-F_i,\quad W_i=\frac{w}{H}\frac{\partial c_i}{\partial\eta}$$

/1054

All equations of this form for the various surfaces of interpolation are related through the derivatives with respect to η; the latter appear in the quantities Φ_i and are determined by (2.3). In general, the approximating system will consist of $(m+5)(l+1)-2$ equations in x and ϑ for the corresponding number of values of functions of all surfaces $\eta=\eta_k$ that are being considered.

In the region in which $u^2+(v+\mu w)^2(1+\mu^2)^{-1}>a^2$, the thus generated approximating system is hyperbolic. This system has two families of characteristics with

$$\frac{d\vartheta}{dx}=\frac{1}{\varepsilon}\left(\lambda+\frac{u^2\zeta-(-1)^i a^2\beta}{u^2-a^2}\right)\equiv A_i. \tag{2.4}$$

On characteristics of the first family (i = 1) and on those of the second family (i = 2), one must satisfy the following relations

$$d\zeta+Kdp+Ldx=0,\quad d\zeta-Idp+Ndx=0. \tag{2.5}$$

In (2.4) and (2.5), we introduced the notation

$$\zeta = \frac{v + \mu w}{Hu}, \quad \beta = \left[\frac{u^2\zeta^2}{a^2} + \frac{(1+\mu^2)}{H^2}\left(\frac{u^2}{a^2} - 1\right)\right]^{1/2},$$

$$L = \Phi_1 \frac{a^2(\zeta + \beta)}{u(u^2 - a^2)} - \Phi_2 \frac{A_1\varepsilon - \lambda}{u^2} + Z,$$

$$N = \Phi_1 \frac{a^2(\zeta - \beta)}{u(u^2 - a^2)} - \Phi_2 \frac{A_2\varepsilon - \lambda}{u^2} + Z,$$

$$Z = \frac{1}{H}\left(\frac{\Phi_3 + \mu\Phi_4}{u^2} - \frac{w}{u}\frac{d\mu}{dx} + \zeta\frac{dH}{dx}\right), \quad I = K = \frac{\beta}{\rho u^2},$$

The approximating system also incorporates a family of analogues of the streamlines, determined by

$$\frac{d\vartheta}{dx} = \frac{1}{\varepsilon}(\lambda + \zeta) \equiv A_3. \tag{2.6}$$

Along these "streamlines,"

$$\begin{aligned} &Bdv - dw + Cdx = 0, \quad du + Gdv + Pdp + Qdx = 0, \\ &dT + gdp + Ddx = 0, \quad dc_i + E_i dx = 0 \quad (i = 1, 2, \ldots, m), \end{aligned} \tag{2.7}$$

where

$$B = \mu, \quad C = \frac{1}{u}(\mu\Phi_3 - \Phi_4), \quad G = H\zeta, \quad P = \frac{1}{\rho u},$$

$$Q = \frac{1}{u}(\Phi_2 + H\zeta\Phi_3), \quad D = \frac{\Phi_5}{u}, \quad E_i = \frac{\Phi_{5+i}}{u},$$

and g has the same meaning as in (1.8). Note that the first two relations of (2.7) can yield an analogue of Bernoulli's equation. /1055

3. Computational algorithms of the method of characteristics

To integrate the approximating system, we apply the numerical scheme of the method of characteristics in which the solution is constructed on successive layers, namely, the planes x = const. On each such plane, we consider a difference grid with nodes formed by the intersection of the surfaces $\eta = \eta_k$ (for k = 0, 1, ..., l) and the surfaces $\vartheta = \vartheta_n$ (for n = 0, 1, ..., n). From these nodes, we draw the characteristics and the "streamlines" in the upstream direction along the flow, until they meet the previous layer, where all the gasdynamic functions are already known. The compatibility relationships represented in finite-difference form along these curves enable us to determine the desired functions at the nodal points of the new layer.

Such a numerical scheme of the inverse type has some advantages over the classical scheme of the method of characteristics, in which the characteristics are drawn in the downstream direction along the flow. In the scheme of the inverse type, the nodes are located at prefixed points, which is convenient from the practical point of view and it makes it possible to fairly simply relocate the nodes during the course of solution.

This last point is especially important in the calculation of nonequilibrium flows when, in small characteristic periods of time, the physicochemical processes take place in a narrow zone adjacent to the shock wave and characterized by large gradients. To achieve accurate results in this zone it is necessary to establish a larger number of nodes than in the remaining region. However, the conditions of numerical stability then also require us to establish more layers x = const. In the characteristic scheme of the inverse type, where all the points with common value $\vartheta = \vartheta_n$ are calculated independently of the other points, this number of layers needs to be increased only in the narrow zone indicated above, and not over the entire flow. This causes a considerable economy in machine time. We note that, in numerical methods where the sweep is applied in the region between the body and the shock wave, such a convenient procedure is impossible.

In a numerical scheme that uses the characteristic relations as difference relationships, the number of variables from which the approximate finite-difference representation of the equations is made decreases by 1. The semi-characteristic scheme developed above differs in its notable simplicity which is due to the reduction of the three-dimensional problem to a two-dimensional one. The present scheme is implicit and can be of second-order accuracy, which facilitates the achievement of stability and increases the efficiency of the scheme. We shall now give the computational algorithms that are used in this scheme for nodes of various types. Because of the implicitness of the scheme, the numerical procedure includes an iterational process. In each individual iteration, a given algorithm is used to calculate simultaneously all 1 + 1 nodes having the same coordinates ϑ and lying on different surfaces $\eta = \eta_k$. The calculations are similar for each surface $\eta = \eta_k$. Therefore, we shall describe them only for a single surface. /1056

In the determination of the functions at a new interior point 0 lying on the layer $x = x_* + \Delta x$, the characteristics of the first and second families (2.4) and the "streamline" (2.6) are drawn from it. They intersect the preceding layer $x = x_*$ at the points 1, 2, and 3, respectively, whose coordinates are

$$\vartheta_i = \vartheta_0 - A_i \Delta x \qquad (i = 1, 2, 3).$$

At these points we can, with the aid of interpolations with respect to one variable, find the values of u, v, w, p, T, and c_i, which we shall indicate by the corresponding numerical subscripts. Then, we shall represent in finite difference the compatibility relations (2.5) along the characteristics and the relations (2.7) along the "streamlines."

Solving the equations thus obtained, we obtain the following computational algorithm:

$$
\begin{aligned}
&p_0 = p_1 + \frac{1}{K+I}[\zeta_1 - \zeta_2 - I(p_1 - p_2) + (N-L)\Delta x],\\
&\zeta_0 = \zeta_1 - K(p_0 - p_1) - L\Delta x, \qquad T_0 = T_3 - g(p_3 - p_0) + D\Delta x,\\
&w_0 = \frac{B\{H_0\zeta_0[u_3 - P(p_0 - p_3) - Q\Delta x] - v_3\} + (1 \pm GH_0\zeta_0)(w_3 + C\Delta x)}{1 + GH_0\zeta_0 + B\mu_0},\\
&u_0 = \frac{1}{1 + GH_0\zeta_0}[u_3 - P(p_0 - p_3) - Q\Delta x + G(v_3 + \mu_0 w_0)],\\
&v_0 = u_0 H_0\zeta_0 - \mu_0 w_0, \qquad c_{i0} = c_{i3} - E_i\Delta x.
\end{aligned}
\tag{3.1}
$$

From these equations we calculate one after the other all the basic functions at the new nodal 0. Here, we must use the equation of state, the expression for the enthalpy (1.2), and the formula for the velocity of sound (1.7).

The coefficients of (2.4)-(2.7) that appear in (3.1) are averaged over the points 0 and 1, 0 and 2, and 0 and 3, respectively. The derivatives with respect to η, which are contained in the quantities Φ, are calculated from (2.3). We note that these derivatives, as well as the coefficients A_i, are found in the first iteration from the values of the functions at the point 4 on the layer $x = x_k$, at which point $\vartheta_4 = \vartheta_0$.

Averaging of all coefficients is done according to the general formula

$$K_{cp} = sK_0 + (1 - s)K_t, \tag{3.2}$$

where s is a weighting parameter. We shall address ourselves later to the choice of this parameter.

If the point 0 to be calculated is on a solid wall, then the compatibility relation (2.5) is computed only along the characteristic of the second family 0-2 and we also use the condition of impenetrability (1.5). In this case, the pressure p_0 and the quantity ζ_0 are calculated from the expressions

$$p_0 = p_2 + \frac{1}{I}(\zeta_0 - \zeta_2 + N\Delta x), \qquad \zeta_0 = -\lambda_0. \tag{1057}$$

For all the remaining functions, the corresponding equations of the system (3.1) remain valid.

Finally, let us look at the determination of a new point 0 on a shock wave. Here, the solution consists primarily of finding the derivative ξ'_{nx}. When we have some value for ξ'_{nx} at the point 0 and take the value of $\xi'_{n\eta}$ from the preceding

layer (it remains constant in the course of the first iteration), we can use formulas (1.6) to find all functions at the point 0. Let us calculate the coordinate of the shock wave ξ_B, using the adjacent wave point 4 on the layer $x = x_*$. We have, specifically,

$$\xi_{B0} = \xi_{B4} + [s(\xi'_{Bx})_0 + (1-s)(\xi'_{Bx})_4]\Delta x_*$$

Now from the point 0, we draw the characteristic of the first family, intersecting the layer $x = x_*$ at point 1. By virtue of the satisfaction of the compatibility relation along this characteristic

$$\zeta_0 - \zeta_1 + K(p_0 - p_1) + L\Delta x = 0$$

a check of the given quantity ξ'_{Bx} is made, and its proper value is fitted with the necessary degree of accuracy. After the first iteration for the entire new layer from the values obtained for ξ_{B0} at various $\eta = \eta_k$, we find, by means of (2.3), the derivative $\xi'_{B\eta}$, which is used in the next iteration.

Let us now pause briefly to look at the stability of the numerical scheme. Here, the Courant-Friedrichs-Levy stability condition can be satisfied by an appropriate choice of steps and method of interpolation on the preceding layer. However, the given characteristic numerical scheme is nonsimplicial. Therefore, it must be checked for Neumann's stability criterion. For this scheme, such an investigation of stability was made by Yu. Ya. Mikhayalov on the linearized equations of gasdynamics. He has shown that the value of the weighting parameter $s = 0.5$ in (3.2) for averaging of the coefficients (that is, in the case in which the scheme has second-order accuracy) corresponds to the stability limit in the sense of Neumann. Consequently, to create a margin of stability, we need to use a somewhat larger value of the weighting parameter, for example, $s = 0.6$, which decreases the order of accuracy of the scheme only to an insignificant extent in comparison with the second order of accuracy.

It is well known that in the calculation of flows with nonequilibrium physical-chemical processes, difficulties arise in those regions where the parameters of the flow are close to equilibrium. Here, the stability of the calculations deteriorates because, under equilibrium conditions, $\varphi_i \to \infty$ and $f_i \to 0$ in the kinetic equation (1.3). In this case, the application of explicit schemes for numerical integration becomes practically impossible because they require an exceptionally small computational step. Implicit schemes which use the behavior of the kinetic equations near the equilibrium enable us to remove this difficulty. In [9, 10, 12, 13], effective numerical schemes were also proposed for calculating two-dimensional gas flows accompanied by fast nonequilibrium processes. /1058

An analogous scheme of the implicit type was used to solve the present three-dimensional problem. This scheme is based on the representation of the function f_i by two terms of the series with respect to the same parameter c_j, which approaches the equilibrium value. As a result, to calculate this parameter c_j at the point 0, we obtain the following difference formula:

$$c_{j0} = c_{j3} + \Delta x \left[(1-s) \frac{F_{j3} - W_{j3}}{u_3} + s \frac{\varphi_{j0} f_{j*} - W_{j0}}{u_0} \right] \times$$
$$\times \left\{ 1 - s \frac{\varphi_{j0} \Delta x}{u_0} \left[(1-s) \left(\frac{\partial f_j}{\partial c_j} \right)_* + s \left(\frac{\partial f_j}{\partial c_j} \right)_0 \right] \right\}^{-1},$$

where the asterisk subscript means that, in the calculation of the corresponding function, the independent variables p, T, and c_i (for $i \neq j$) are taken at the point 0 in question and the parameter c_j is taken at the preceding point 3 on the streamline. At s = 0.5 this difference formula is of second-order accuracy and enables us to calculate in a unique way the gas flow in regions both near and far from the equilibrium. Thus, this general formula should be applied in (3.1) instead of the last formula, which is not suitable for calculating nonequilibrium processes with very small characteristic times.

4. Supersonic flow in nonaxisymmetric nozzle

The numerical method that we have developed was applied to the solution of the specific problem of calculating the nonequilibrium three-dimensional supersonic flow of a gas in a nonaxisymmetric annular nozzle.

The outer wall of this nozzle was a cylinder of elliptical cross-section with semi-axis ratio a/b = 1.5 and with a = 50 cm. The internal body in the nozzle has the following geometry. In the plane of symmetry, in which the major semiaxis a lies, the contour of the interior body is a part of the Joukowski profile and is given by equations in parametric form

$$x = A(r + 1/r)\cos\gamma - x_0, \quad y = A(r - 1/r)\sin\gamma,$$

where

$$r = -\varepsilon\cos\gamma + (1 + 2\varepsilon + \varepsilon^2\cos^2\gamma)^{1/2},$$

and the x-axis coincides with the axis of the nozzle. We assumed a profile for which A = 167, ε = 0.125, and the quantity x_0 is such that, in the initial section of the nozzle (x = 0), the tangent to the profile is parallel to the axis of the nozzle.

The cross sections of the internal body in every plane x = const are ellipses with the same focal distance and the same major semi-axis, equal to the coordinate y(x) of the chosen Joukowski profile. In the initial plane x = 0, the cross-section of the internal body is an ellipse with the same ratio a/b = 1.5 as in the external cylindrical tube. It is with just this ellipse that the variables ξ and η for the entire region of flow are connected, and the linear results apply to half its focal distance δ = 36.2 cm. For this ellipse, we have $\xi = \tanh^{-1}(b/a)$. We refer the values $\eta = 0°$ and $\eta = 90°$ to the planes of symmetry in which the minor and major semiaxes lie respectively. In this coordinate system, the cross-section of the interior body is, in every plane x = const, determined by $\xi = \xi(x) =$ = const. In particular, the annular cross-section degenerates to a straight line segment ($\xi = 0$). /1059

The form of the nozzle in question in the two planes of symmetry $\eta = 0°$ and $\eta = 90°$ is shown in Fig. 1.

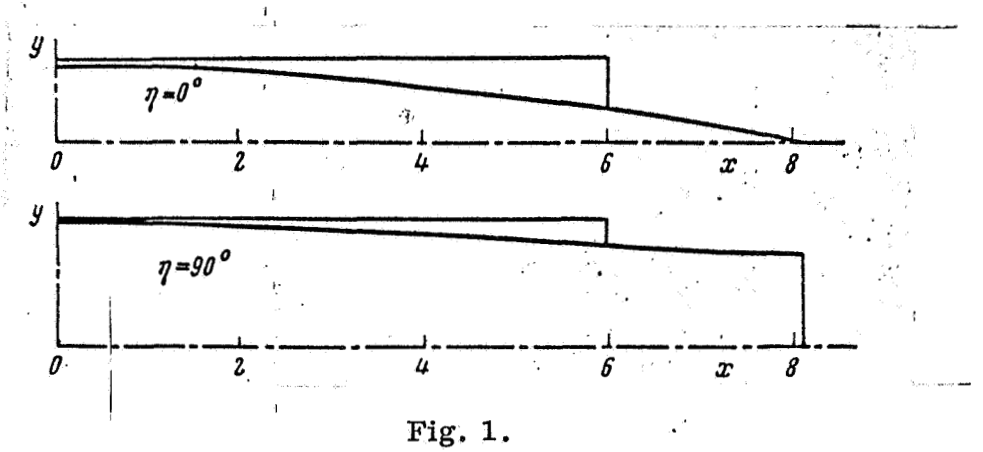

Fig. 1.

In the initial cross-section of the nozzle, we are given a uniform supersonic flow of gas with velocity vector parallel to the axis of the nozzle. We assume that the gas is in a state of thermodynamic equilibrium. We shall characterize this flow by three gasdynamic parameters, namely, the velocity V_∞ (or the Mach number M_∞), the pressure p_∞, and the temperature T_∞.

Calculations of the three-dimensional flow in an annular non-axisymmetric nozzle were made, just as in [9, 10] in the axisymmetric case, for oxygen in nonequilibrium dissociation when there are equilibrially excited translational, rotational, and vibrational degrees of freedom and when there are no excited electronic levels and no ionization. Then, the role of the nonequilibrium parameter will be played by the degree of dissociation, that is, the ratio of the mass of atomic oxygen to its entire mass. All equations related with the physical kinetics are borrowed from [10].

The equation of state and the expression for the enthalpy (1.2) for a diatromic gas is taken in the dimensionless form

$$\rho = \frac{p}{T}(1+c), \qquad h = \frac{7+3c}{2}T + \Theta_D c + (1-c)\Theta_v \frac{\exp(-\Theta_v/T)}{1-\exp(-\Theta_v/T)} \tag{4.1}$$

The functions φ and f in (1.4), the product of which constitutes the right side of an equation for the degree of dissociation of the type (1.3), have the form

$$\varphi = \frac{\Lambda\rho}{T^l(1+c)}\left[2c + \frac{k_{R2}}{k_{R1}}(1-c)\right],$$
$$f = \omega(1-c^2)\sqrt{T}\left[1-\exp\left(-\frac{\Theta_v}{T}\right)\right]\exp\left(-\frac{\Theta_D}{T}\right) - \frac{pc^2}{T}. \tag{4.2}$$

Equations (4.1) and (4.2) have the following dimensionless parameters, which are combinations of the dimensional quantities

$$\Theta_D = \frac{T_D R}{V_\infty^2}, \quad \Theta_v = \frac{T_v R}{V_\infty^2}, \quad \omega = \frac{\rho_D V_\infty}{\rho_\infty T_D^{1/2} R^{1/2}}, \quad \Lambda = \frac{k\delta\rho_\infty^2 R^l}{\mu^2 V_\infty^{1+2l}}.$$

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Here, the physical constants have the following meanings: R is the gas constant of the undissociated gas, μ is the atomic weight, T_v is the characteristic vibrational temperature, T_D is a constant proportional to the energy of dissociation of the molecule, ρ_D is a constant with the dimensions of density, k_{R1} and k_{R2} are the constants of speed of recombination in the case of a triple collision, and, in particular, $k_{R1} = kT^{-l}$. For oxygen, these constants were taken as follows: $R = 2.6 \cdot 10^6$ cm^2/sec^{2}deg, $\mu = 16$ g/g-mole, $T_v = 2256°$ K, $T_D = 59,370°$ K, $\rho_D = 1540$ g/cm^3, $k = 4.8 \cdot 10^{18}$ cm^{6}deg/sec-g-mole^2, $k_{R1}/k_{R2} = 3$, and $l = 1$.

Let us give some results of calculations of supersonic flow of nonequilibrially dissociating oxygen in a nozzle of the given form. The flow at the entrance section of the nozzle had Mach number $M_\infty = 1.2$ and temperature $T_\infty = 5000°$ K, and the value of the pressure p_∞ varied from one variant to another. The graphs given below show the distribution of a number of physical parameters on the inner surface of an elliptic tube bounding the nozzle from the outside. To estimate the accuracy of the numerical solution, calculations were made with a different number of terms in the approximating trigonometric polynomials (2.2). Accordingly, in the region $0° \leqslant \eta \leqslant 180°$, we took five and nine surfaces of interpolation $\eta = \text{const}$. The data found for the first case is indicated on the graphs by circles, that for the second by curves. In all calculations, we considered 25 nodes on each surface $\eta = \text{const}$.

The results of the calculations by use of approximating polynomials of various orders are shown in Figs. 2-4. Here, the pressure was taken equal to $p_\infty = 10$ atm. Figure 2 shows the distribution of the degree of dissociation c and of the relative temperature T/T_∞ along two generators of the nozzle lying in the planes of symmetry $\eta = 0°$ and $\eta = 90°$. The dependence of the relative pressure p/p_∞ on the coordinate η for a number of values $x = \text{const}$ is shown by the solid curve in Fig. 3. As one can see, the accuracy in the determination of the degree of dissociation, temperature, and pressure is good even when there are only a small number of surfaces of interpolation.

However, in three-dimensional flows, the circular component of the velocity w is a more sensitive function, in the sense of accuracy of numerical solution. The change in this quantity along the generator of the nozzle $\eta = 45°$ is shown in Fig. 4, which shows the data calculated at a different degree of accuracy. It turns out that, for large distances x, five surfaces of interpolation $\eta = \text{const}$ are not enough for satisfactory determination of the angular velocity w.

It is of interest to juxtapose nonequilibrium flow of oxygen in a nozzle with the corresponding limiting flows that is, with equilibrium dissociation and "frozen

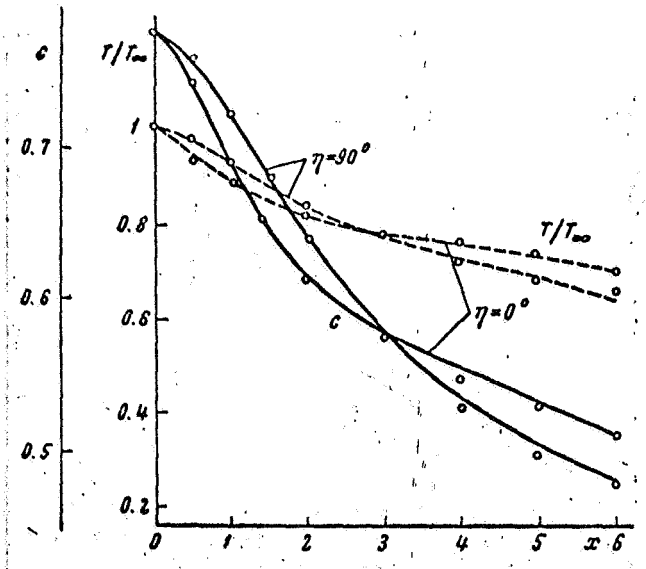

Fig. 2.

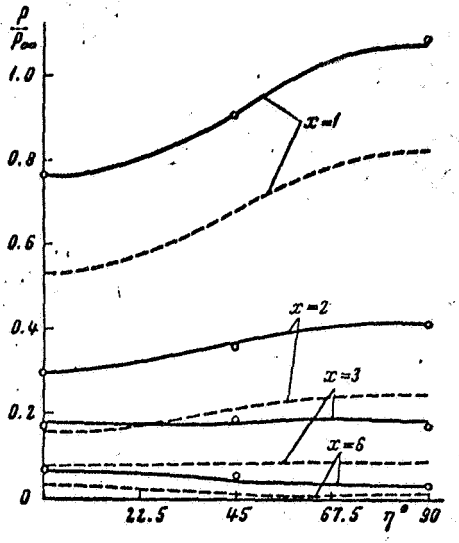

Fig. 3.

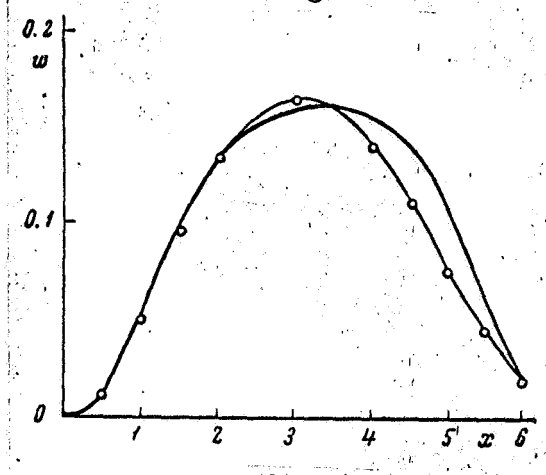

Fig. 4.

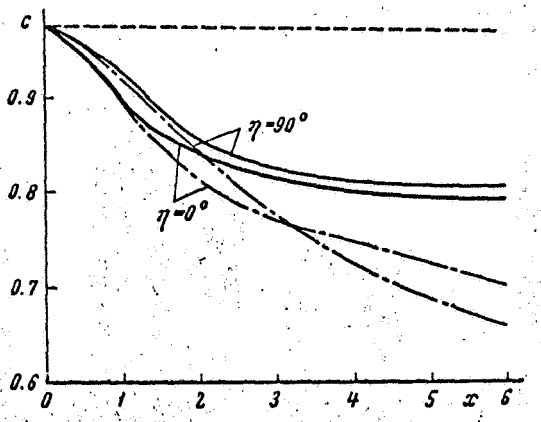

Fig. 5.

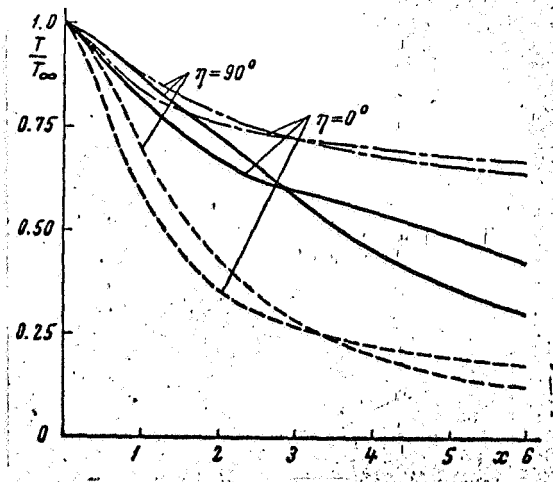

Fig. 6.

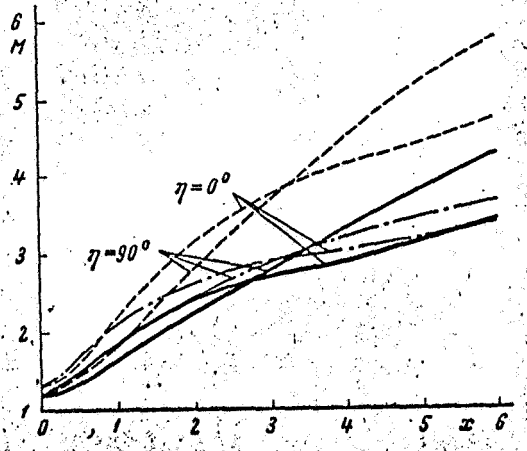

Fig. 7.

in" dissociation. This comparison is made in Figs. 5-7. The results, pertaining to the nonequilibrium, equilibrium, and "frozen-in" cases are shown by the solid, short-and-long-dash, and medium-dash curves respectively. In all these /1062
cases, the incident flow had the same pressure p_∞ (namely, 1 atm) and the same velocity V_∞. Here, for the equilibrium flow, the Mach number M_∞, calculated from the equilibrium velocity of sound, was equal to $M_\infty = 1.316$.

The distribution of the degree of dissociation c along the length of the nozzle for $\eta = 0°$ and $\eta = 90°$ is shown in Fig. 5. In the nonaxisymmetric nozzle under consideration, the nature of the change of this quantity is the same as in an axisymmetric nozzle. In the initial region, the curves representing the degree of dissociation in a nonequilibrium process are close to the curves representing an equilibrium dependence. In further sections, the flow deviates from an equilibrium state and becomes "frozen-in" rather rapidly. Here, the degree of dissociation remains virtually constant, though not the same, for the different surfaces $\eta = \text{const}$.

The graphs shown in Figs. 6 and 7 give the change in the temperature T/T_∞ and the Mach number M along the outer wall of the nozzle for the three types of flow mentioned above. Furthermore, Fig. 3 shows (the dashed curves) the distribution of the pressure in the "frozen-in" case. These numerical results emphasize that analysis of the nonequilibrium dissociation, with finite rates of this process, is of significance and that it influences most of all the temperature of the flow.

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